

Metal-insulator transition in disordered 2DEG including temperature effects.

J.S. Thakur^{*}, Lerwen Liu[†] and D. Neilson^{*†}

^{*}*School of Physics, The University of New South Wales, Sydney 2052, Australia*

[†]*Scuola Normale Superiore, Piazza dei Cavalieri 7, 56126 Pisa, Italy*

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We calculate self-consistently the mutual dependence of electron correlations and electron-defect scattering for a two dimensional electron gas at finite temperature. We employ an STLS approach to calculate the electron correlations while the electron scattering rate off Coulombic impurities and surface roughness is calculated using self-consistent current-relaxation theory. The methods are combined and self-consistently solved. We discuss a metal-insulator transition for a range of disorder levels and electron densities. Our results are in good agreement with recent experimental observations.

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In recent experiments [1–3] on two-dimensional electronic systems in zero magnetic field a well defined metal-insulator transition has been observed. The transition contradicts the prediction [4] that two dimensional electron systems are always localized in the presence of any disorder. The mobility is large at the transition point ($\mu > 1\text{m}^2/\text{Vs}$). For such a high mobility the scattering off defects will be weak and electron correlations could make a significant difference.

Both disorder and correlations by themselves can lead to at least two different types of localization. In the presence of disorder Abrahams *et al* [4] showed that non-interacting electrons in two dimensions cannot sustain static conductivity no matter how small the level of disorder is. On the other hand if there are strong correlations between the charge carriers this can cause a different type of localization in disorder-free systems which is associated with Wigner crystallization [5]. In real systems there are both electron-electron and electron-impurity interactions. With weak disorder and in the low electron density limit the electron-electron interactions should dominate leading to Wigner crystallization, while in the high electron density limit the electron correlations are very weak and the localization should be of the Anderson type. Between these two extremes disorder and correlations compete with each other to decide the nature of the localization.

In this paper we examine the interdependence of correlations and defect scattering at finite temperatures. We use the self-consistent formalism of Singwi, Tosi, Land and Sjölander (STLS) [6] to treat electron-electron correlations, while for the electron-defect scattering we use a memory function approach [7] to calculate the decay time of the density fluctuations from scatterings off defects. Previous calculations of the influence of disorder have either used the first Born approximation or else they have introduced an adjustable parameter γ for the electron scattering rate from the disorder. In these approaches the scattering rate is not affected by correlations while the two effects are in fact interdependent and should be

self-consistently linked.

We consider a random distribution of Coulombic impurities with charge e and density n_i . The charge carrier (electron or hole) density n_c is chosen low enough that the carriers occupy only the lowest energy subband. In the STLS formalism the bare Coulomb potential $V(q) = 2\pi e^2/q\epsilon$ acting between the carriers is replaced by an effective interaction $V_{\text{eff}}(q) = V(q)[1 - G(q)]$, where $G(q)$ is a local field factor. $V_{\text{eff}}(q)$ is generally weaker than $V(q)$ because of the correlations between the carriers. The response function becomes

$$\chi(q, \omega) = \frac{\chi^{(0)}(q, \omega)}{1 + V(q)[1 - G(q)]\chi^{(0)}(q, \omega)}. \quad (1)$$

We include the effect of disorder by replacing the free particle dynamical susceptibility $\chi^{(0)}(q, \omega)$ in Eq. 1 by the response function for non-interacting charge carriers scattering from the disorder [8],

$$\chi^{(s)}(q, \omega) = \frac{\chi^{(0)}(q, \omega + i\gamma)}{1 - \frac{i\gamma}{\omega + i\gamma} \left[1 - \frac{\chi^{(0)}(q, \omega + i\gamma)}{\chi^{(0)}(q)} \right]}. \quad (2)$$

$\chi^{(0)}(q, \omega + i\gamma)$ is the susceptibility for non-interacting carriers scattering off the disorder. We use the memory function formalism [9] to calculate the scattering rate γ . This is related to the mobility μ by the Drude expression $\mu = e/m^*\gamma$. At zero temperature in the diffusive regime $\chi^{(s)}(q, \omega)$ is given by $\lim_{\omega, q \rightarrow 0} \chi^{(s)}(q, \omega) = (2m^*)/(\pi k_F \hbar^2)(\mathcal{D}q^2)/(\mathcal{D}q^2 + i\omega)$, where $\mathcal{D} = v_F^2/\gamma$ is the diffusion constant. In the limit when γ goes to infinity the system becomes non-diffusive. This represents a localized phase [10].

In the memory function formalism γ is expressed in terms of the non-linear equation [7]

$$i\gamma = -\frac{1}{2m^*n_c} \sum_q q^2 [\langle |U_{\text{imp}}(q)|^2 \rangle + \langle |W_{\text{surf}}(q)|^2 \rangle] \times \left(\frac{\tilde{\chi}(q)}{\chi^{(0)}(q)} \right)^2 \Phi(q, i\gamma) \quad (3)$$

$$\Phi(q, i\gamma) = \frac{\phi_0(q, i\gamma)}{1 + i\gamma\phi_0(q, i\gamma)/\chi^{(0)}(q)}. \quad (4)$$

$\Phi(q, i\gamma)$ is the relaxation spectrum for non-interacting carriers that scatter off the disorder with scattering rate γ . It is expressed in terms of $\phi_0(q, i\gamma) = (1/i\gamma) [\chi^{(0)}(q, i\gamma) - \chi^{(0)}(q)]$ which is the relaxation function for non-interacting carriers with lifetime γ^{-1} . The static response function $\tilde{\chi}(q) = \chi^{(0)}(q)/\{1 + V(q)[1 - G(q)]\chi^{(0)}(q)\}$ includes the correlations between the carriers for the disordered system. $U_{\text{imp}}(q) = [(2\pi e^2)/(\epsilon q)] \exp(-qd)F_i(q)$ is the impurity potential for the monovalent Coulomb impurities which are in a layer separated from the electron or hole plane by a distance d . We use for the impurity form factor $F_i(q)$ Eq. 4.28 in Ref. [11]. For electrons in the Si MOSFETs we also include interface surface roughness scattering. This is the term $W_{\text{surf}}(q) = \sqrt{\pi}\Delta\Lambda\Gamma(q)\exp(-(q\Lambda)^2/8)$. Values for the parameters $\Lambda = 0.37\text{nm}$ and $\Delta = 2.0\text{nm}$ are taken from Si MOSFET data [12]. For $\Gamma(q)$ we use the expression in Ref. [13]. For GaAs surface roughness scattering is much smaller and we set $W_{\text{surf}}(q) = 0$.

In the STLS formalism the density-density correlation function $\langle\delta\hat{n}(r, t)\delta\hat{n}(r', t)\rangle$ is approximated by the non-linear product, $\delta n(r, t) \times g(r - r') \times \delta n(r', t)$. The $\delta n(r, t)$ are expectation values and $g(r)$ is the pair-correlation function giving the probability of finding electrons a distance r apart. Using $g(r) = 1 + n_c^{-1} \int d^2\mathbf{q} \exp(i\mathbf{q}\cdot\mathbf{r})[S(q) - 1]$, this gives us a relation between the static structure factor $S(q)$ and the local field factor $G(q)$,

$$G(q) = -\frac{1}{n_c} \int \frac{d^2\mathbf{k}}{(2\pi)^2} \frac{(\mathbf{q} \cdot \mathbf{k})}{q^2} \frac{V(\mathbf{k})}{V(\mathbf{q})} [S(|\mathbf{q} - \mathbf{k}|) - 1]. \quad (5)$$

For a given $G(q)$ we can determine γ from Eq. 4. Then $S(q) = (n_c\pi)^{-1} \int_0^\infty d\omega \text{Im}\chi(q, \omega)$ is calculated from the fluctuation-dissipation theorem and

$$\chi(q, \omega) = \frac{\chi^{(s)}(q, \omega)}{1 + V(q)[1 - G(q)]\chi^{(s)}(q, \omega)}. \quad (6)$$

Equation 5 gives a new local field factor which can be used in Eq. 4. The process is repeated iteratively until there is overall self-consistency with both γ and $G(q)$.

Our variables are the carrier density n_c , the impurity density n_i , and the distance separating the impurities from the electron or hole plane d . The Metal Insulator Transition is observed at carrier densities that are relatively low by conventional semiconductor standards so the Fermi temperature $T_F = E_F/k_B$ can be of the order of a few degrees K. We have solved the equations at finite temperatures and determined the dependence of γ on temperature up to $T \lesssim T_F$.

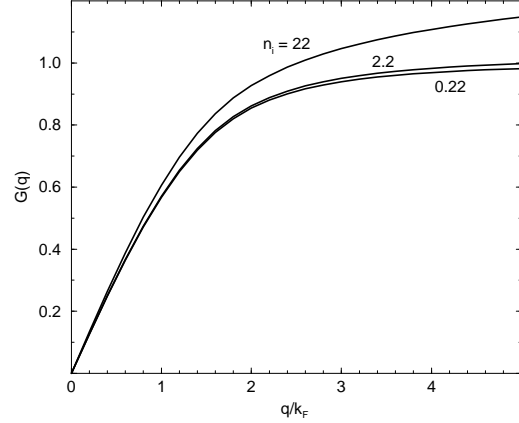


FIG. 1. Local-field-factor $G(q)$ for different impurity densities. The impurities are separated from the carrier plane by $d=5a_0^*$. Carrier density is $n_c = 35 \times 10^{10} \text{cm}^{-2}$.

Figure 1 shows the dependence of the local field factor $G(q)$ on the impurity concentration at zero temperature. Increasing the disorder enhances $G(q)$. This is caused by the decrease in $\chi^{(s)}$ as the scattering rate γ gets bigger (Eq. 2). Enhancing $G(q)$ weakens the effective interaction between the carriers, and hence weakens the screening of the carrier-impurity potential. The net result of enhancing $G(q)$ is thus to strengthen the effect of the disorder potential. This in turn further increases γ . At a critical level of disorder this non-linear feedback causes γ to increase rapidly and leads to localization of the carriers.

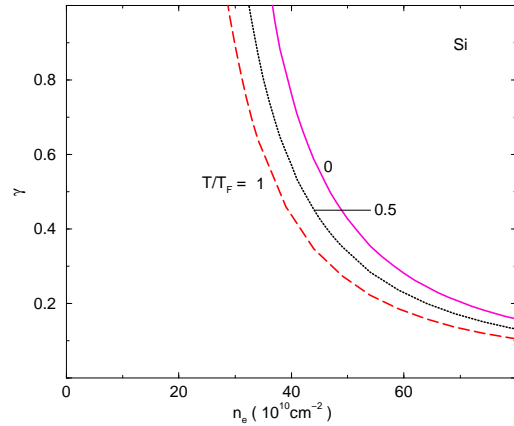


FIG. 2. Scattering rate γ for Si as a function of electron density for impurity density $0.5 \times 10^{11} \text{cm}^{-2}$. Separation of the impurity layer is $d=a_0^*$. Curves are for temperatures T (labels are in units of the Fermi temperature T_F for density n_c).

We see this non-linear behavior in Fig. 2. At a certain critical carrier density the scattering rate γ starts to increase rapidly. The impurity density here is $n_i =$

$0.5 \times 10^{11} \text{cm}^{-2}$, with the impurities separated from the carrier plane by distance $d = a_0^*$ (a_0^* is the effective Bohr radius). The non-linear increase in γ is due (i) to the enhancement of the local field $G(q)$ which strengthens the disorder potential, and (ii) to the rapid increase in the relaxation spectrum $\Phi(q, i\gamma)$ with γ . Figure 2 also shows the dependence of γ on temperature. The labels on the curves give the temperature in units of T_F for density n_c . γ diminishes with increasing temperature. This reflects the weakening of the correlations at finite T .

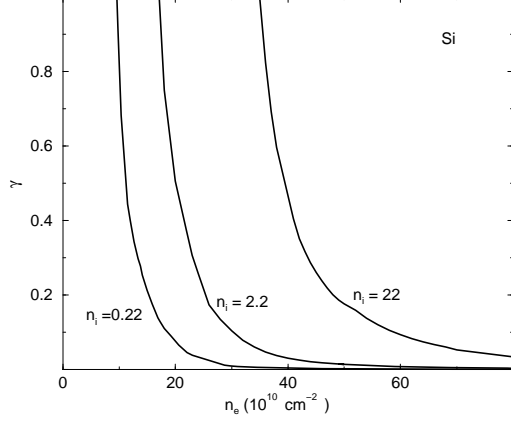


FIG. 3. Scattering rate γ for Si at $T = 0$ as a function of electron density. Curves are labelled for different impurity densities n_i (in units of 10^{11}cm^{-2}). Impurity separation $d = 5a_0^*$.

In Figure 3 we show the increase of γ with impurity density at $T = 0$. The curve labels give n_i in units of 10^{11}cm^{-2} . The impurity separation is $d = 5a_0^*$. As expected, increasing the impurity concentration has the effect of increasing the scattering rate. On the other hand, increasing the carrier density has the opposite effect on γ because the correlations are reduced. However the non-linear effects from n_c are much stronger than the non-linear effects from n_i .

There exists no first order localization-delocalization transition in two-dimensions. In the metallic phase the mean-free-path is large $\ell k_F \gg 1$ while in the localized phase ℓk_F should be $\lesssim 1$. We take the localization boundary to be the point where $\ell k_F = 1$. Table I gives for different temperatures the critical electron density at which ℓk_F passes through unity. When the system is at finite temperature the correlations are reduced and one needs to go to slightly lower carrier densities before localization can be achieved.

Table I shows the temperature dependence is quite small and so we give Metal-Insulator phase diagrams for $T = 0$. The dependence of the hole density at the transition on the impurity layer separation d for GaAs is shown in Fig. 4. The impurity density is fixed at $n_i = 0.5 \times 10^{11} \text{cm}^{-2}$. We compare our results with the

observation of the transition in Ref. [3] in a GaAs sample. Our curve is consistent with this measurement. The phase boundary is sensitive to d because of the exponential factor in $U_{\text{imp}}(q)$. This suppresses carrier-impurity scattering for short wavelengths $q \gg d$. For the residual long wavelength scattering the correlations are always weak. Thus when d is large the correlations play a relatively less important role in the localization.

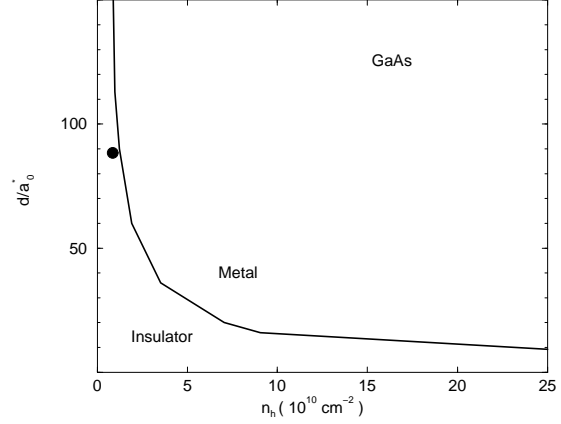


FIG. 4. Phase diagram for holes in GaAs. Critical hole density n_h at which $\gamma = 1$ as a function of impurity layer separation d . Impurity density is $n_i = 22 \times 10^{11} \text{cm}^{-2}$. The experimental data point for GaAs is from Ref. [3].

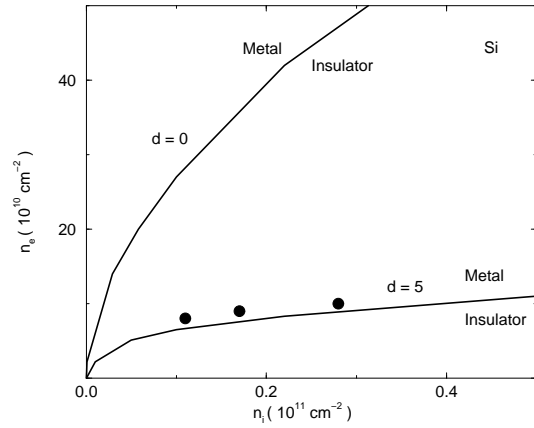


FIG. 5. Phase diagram for electrons in Si. Critical carrier density at which $\gamma = 1$ as a function of impurity density for separations $d=0$ and $5a_0^*$. The experimental data points are taken from Ref. [2].

The phase diagram in Figure 5 plots the critical electron density in Si at the transition as a function of impurity density n_i . The impurity layer separations are $d = 0$ and $5a_0^*$. We also show experimental data points for the position of the Metal-Insulator transition in Si

[2]. Again our predicted phase boundary agrees with these observations. On our curve the electron-impurity scattering becomes weaker as the critical electron density decreases. Thus at the transition point the electron mobility will increase as the electron density decreases. This is consistent with recent observations [2].

We conclude that correlations and impurity scattering do mutually affect the localization transition. Finite temperatures tend to suppress correlations and this slightly reduces the critical carrier density for localization to occur by an amount which becomes significant for temperatures of the order T_F .

ACKNOWLEDGMENTS

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| T (K) | 0 | 1 | 10 | 20 |
|----------------------------|---------------------|---------------------|---------------------|---------------------|
| n_e (cm^{-2}) | 37×10^{10} | 37×10^{10} | 32×10^{10} | 29×10^{10} |

Table I

Dependence on temperature of the critical carrier density for localization in Si. Impurity density $n_i = 0.5 \times 10^{11} \text{cm}^{-2}$. Impurities are embedded in the carrier plane.

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